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And your equation is equal to E Psi. And we saw that these energies, the binding energies of the electron to the nucleus, were quantized. Well, these energy levels then were given by minus this Rydberg constant R sub H over n squared. And this n was our quantum number. It is a principle quantum number. And we saw that n, the smallest value was 1, 2 and ran all the way up to infinity. Well, today what we are going to do is solve this equation, or we are going to look at the results of solving this equation for the wavefunction Psi. Now, Psi, in general, is the function of r, theta, phi, and also time. But we are going to be looking at problems in which time does not have an effect. In other words, the wave functions that we are going to be looking at are what are called stationary waves. We actually are not going to be looking at the wave function as a chemical reaction is happening. We are either going to look at it before or after, but not during. And, in those cases, we are looking at a wave function. And the atom is just stable and is sitting there. The time dependence here does not have a consequence. And so, therefore, the wave functions that we are going to be looking at are just a function of r, theta and phi. And we are looking at what is called time-independent quantum mechanics. Later on, actually, if you are in chemistry, in a graduate course in chemistry, is when you look at time-dependent wave functions. We are going to look at time-independent quantum mechanics, the stationary wave. Now, it turns out that when we go and solve the SchrÈ†dinger equation here for Psi, what happens is that two more quantum numbers drop out of that solution to the differential equation. Remember, we said last time how quantum numbers arise. They arise from imposing boundary conditions on a differential equation, making that differential equation applicable to your actual physical problem. And so, when we do that, we get a new quantum number called l. And l is, I think you already know, the angular momentum quantum number. Absolutely. It is called the angular momentum quantum number because it indeed dictates how much angular momentum the electron has. It has allowed values. The allowed values of l, now, are zero. Zero is the smallest value of l, the lowest value of l allowed. 1, 2, all the way up to n minus can have. It cannot be any larger than n minus 1. Why can't it be larger than n minus 1? Well, it cannot because the angular momentum quantum number, at least if you want to think classically for a moment, dictates how much rotational kinetic energy you have. And remember that this energy, here, is dependent only on n. This energy is the sum of kinetic energy plus potential energy. If l had the same value as n, well, essentially, that would mean that we would have only rotational kinetic energy and we would have no potential energy. But that is not right. We have potential energy. We have potential energy of interaction. So, physically, that is why l is tied to n. And it cannot be larger than n minus 1. And then, we have a third quantum number that drops out of that solution, which is called M. It is the magnetic quantum number. It is called that because indeed it dictates how an atom moves in a magnetic field. Or, how it behaves in a magnetic field. But, more precisely, m is the z-component of the angular momentum. l is the total angular moment. m dictates the z-component of the angular momentum. And the allowed values of m are m equals zero. You can have no angular momentum in the z-component. Or, plus one, plus two, plus three, all the way up to plus l. Again, m is tied to l. It cannot be larger than l, because if it were then you would have more angular momentum in the z-component than you had total angular momentum. And that is a no-no. So, m is tied to l. The largest value you can have is l. But, since this is a z-component and we've got some direction, m could also be minus 1, minus two, minus three, minus l. We have three quantum numbers, now. That kind of makes sense because we have a 3-dimensional problem. We are going to have to have three quantum numbers to completely describe our system. The consequence, here, of having three quantum numbers is that we now have more states. For example, our n equals 1 state that we talked about last time, more completely we have to describe that state by two other quantum numbers. When n is equal to one, what is the only value that l can have? Zero. And if l is zero, what is the only value m can have? Zero. And so, more appropriately, or more completely, that n equals 1 state is the (1, 0, 0) state. And, if we have an electron in that (1, 0, 0) state, we are going to describe that electron by the wave function Psi(1, 0, 0). Now, what I have not told you yet is exactly how Psi represents the electron. I am just telling you right now that Psi does. Exactly how it does is something I haven't told you yet. And we will do that later in the lecture today, sort of. That is the energy, minus the Rydberg constant. But now, if n is equal two, what is the smallest value that l can have? Zero. And the value of m in that case? Zero. And so our n equals 2 state is more completely the (2, 0, 0) state. And the wave function that describes the electron in that state is the Psi(2, 0, 0) wave function. And then, of course, here is the energy of that state. Now, when n is equal to 2, what is the next larger value of l? One. And if l is equal to one, what is the largest value that m can be? One. And so we have another state here, the (2, 1, 1) state. And if you have an electron in that state, it is described by the Psi(2, 1, 1) wave function. However, the energy here is also minus one-quarter the Rydberg constant. It has the same energy as the (2, 0, 0) state. Now, if n is equal two and l is equal to one, what is the next larger value of m? Zero. And so we have a (2, 1, 0) state. Again, that wave function, for an electron in that state, we label as Psi(2, 1, 0). And then, finally, when n is equal to two, l is equal to one, what is the final possible value of m? Minus one. We have a (2, 1, -1) state and a wave function that is the (2, 1, -1) wave function. Notice that the energy of all of these four states is the same, minus one-quarter the Rydberg constant. These states are what we call degenerate. Degenerate means having the same energy. That is important. Now, this is the way we label wave functions, but we also have a different scheme for talking about wave functions. That is, we have an orbital scheme. And, as I said, or alluded to the other day, an orbital is nothing other than a wave function. It is a solution to the SchrÈ†dinger equation. That is what an orbital is. It is actually the spatial part of the wave function. There is another part called the spin part, which we will deal with later, but an orbital is essentially a wave function. We have a different language for describing orbitals. The way we do this, I think you are already familiar with, but we are going to describe it by the principle quantum number and, of course, the angular momentum quantum number and the magnetic quantum number. Except that we have a scheme or a code for l and m. That code uses letters

instead of numbers. For example, if l is equal to zero here, we call that an s wave function or an s orbital. For example, in the orbital language, instead of Psi(1, 0, 0), we call this a 1s orbital. Here is the principle quantum number. Here is s. l is equal to zero. That is just our code for l is equal to zero. This state, (2, 0, 0), you have an electron in that state. Well, it can describe that wavefunction by the 2s orbital. Here is the principle quantum number. He is s, our code for l equals zero. Now, when n is equal to 1, we call that a p wave function or a p orbital. This state right here, it is the 2p state. Because n is two and l is one, this state is also the 2p wave function and this state, it is also the 2p wave function. Now, if I had a wave function up here where l was equal to two, we would call that d orbital. And, if I had a wave function up here where l was three, we would call that an f orbital. But now, all of these wave functions in the orbital language have the same designation, and that is because we have not taken care of this yet, the m quantum number, magnetic quantum number. And we also have an alphabet scheme for those quantum numbers. The bottom line is that when m is equal to zero, we put a z subscript on the p. When m is equal to zero, that is our 2pz wave function. When m is equal to one, we are going to put an x subscript on the p wave function. And when m is equal to minus one, we are going to put a y subscription on the wave function. However, I have to tell you that in the case of m is equal to one and m is equal to minus one, that is not strictly correct. And the reason it is not is because when you solve SchrÉ†dinger equation for the (2, 1, 1) wave function and the (2, 1, -1) wave function, the solutions are complex wave functions. They are not real wave function. And so, in order for us to be able to draw and think about the px and the py wave functions, what we do is we take a linear combination of the px and the py wave functions. We take a positive linear combination, in the case of the px wave function. The px wave function is really this wave function plus this wave function. And the py wave function is really this wave function minus this wave function. Then we will get a real function, and that is easier to deal with. That is strictly what px and py are. px and py are these linear combinations of the actual functions that come out of the SchrÉ†dinger equation. pz is exactly correct. pz, M is equal to zero, in the pz wavefunction. Now, you are not responsible for knowing that. I just wanted to let you know. You don't have to remember that m equal to one gives you the x subscript, and m equal to minus one gives you the y subscript. You do have to know that when m is equal to zero, you get a z subscript, because that is exactly right. Now, just one other comment here. That is, you see we did not put a subscript on the s wave functions. Well, that is because for an s wave function, the only choice you have for m is zero. And so we leave out that subscript. We never put a z on there or a z on there. It is always 1s, 2s, or 3s. Well, in order to understand that just a little more, let's draw an energy level diagram. Here is the energy again. And for n equals 1, we now see that the more complete description is three quantum numbers, (1, 0, 0). That gives us the (1, 0, 0) state, or sometimes we say the 1s state. There is one state at that energy. But, in the case of n equals 2, we already saw that we have four different states for the quantum number. Four different states. They all have the same energy. They are degenerate. Degenerate means having the same energy. They differ in how much angular momentum the electron has. Or, how much angular momentum the electron would have in the z component if it were in a magnetic field. The total energy is the same because only n determines the energy. It is just that the amount of angular momentum, or the z component of the angular momentum, differs in 2s, 2py, 2pz, 2px, but they all have the same energy. In general, for any value of n, there are n squared degenerate states at each value of n. If we have n is equal to three, then the energy is minus one-ninth the Rydberg constant. But how many states do we have at n equal three? Nine. Here they are. Just like for n equal two, we have the 3s, 3py, 3pz, and 3px. And there are the associated quantum numbers for that. But now we have some states here that I have labeled 3d states. Well, when you have a d state, that means l is equal to two. All of these states have principle quantum number three and angular momentum quantum number two. And they differ also by the amount of angular momentum in the z direction. They differ in the quantum number m. For example, we are going to call the m equal minus two state the 3d(xy). We are going to put xy as a subscript. For m equal minus one, we are going to put a subscript yz. For m equals zero, we are going to put a subscript z squared. For m equal one, d(xz). And for m equal two, x squared minus y squared. Again, for m equal minus two, minus one, one and two, those wave functions, when you solve SchrÉ†dinger equations, are complex wave functions. And what we do to talk about the wave functions is we take linear combinations of them to make them real. And so, when I say m is minus two, is the 3dxy wave function, it is not strictly correct. Therefore, again, you don't need to know m minus two. You don't need to know that subscript. Or m equal one, you don't need to know that subscript. But for m equal zero, this is a z squared. Absolutely. These wave functions are linear combinations. This one is not. It is a real function when it comes out of the SchrÉ†dinger equation. You will talk about these 3d wave functions a lot with Professor Cummins in the second-half of the course. You will actually look at the shapes of those wave functions in detail. So, that's the energy level diagram, here. All right. Now let's actually talk about the shapes of the wave functions. I am going to raise this screen, I think. What do these wave functions actually look like? Well, for a hydrogen atom, our wave function here, given by three quantum numbers, n, l and m, function of r, theta and phi, it turns out that those wave functions are factorable into a function that is only in r and a function that is only in the angles. You can write that, no approximation, this is just the way it turns out. The function that is a function only of r, R of r, is called the radial function. We will call it capital R, radial function of r. It is labeled by only two quantum numbers, n and l. The function that is a function only of the angles, theta and phi, we are going to call Y. This is the angular part of the wave function. And it labeled by only two quantum numbers, but they are l and m. Sometimes we call this angular part, for short, the Y(lm)'s. There is a radial part, and there is an angular part. The actual functional forms are what I show you here on the side screen. And, in this case, what I did is to separate the radial part from the angular part. This first part, here, is the radial part of the wave function. And here on the right is the angular part of the wave function. And I have written them down for the 1s, the 2s, and the bottom one is the 3s, although I left the label off in order to get the whole wave function in there. I want you to notice, here, that the angular part, the Y(lm) for the s wave functions, it has no theta and phi in it. There is no angular dependence. They are spherically symmetric. That is going to be different for the p wave functions. The angular part is just one over four pi to the one-half power. And it is the radial part, here, that we actually are going

to take a look at right now. Let's start with that 1s wave function, up there. If I plot that wavefunction, this is Psi(1, 0, 0), or the 1s wave function versus r. Oh, I should tell you one other thing that I didn't tell you. That is that throughout these wave functions, you see this thing called a nought. a nought is a constant. It is called the Bohr radius. I will explain to you where that comes from in a little bit later. But it has a value of about 0.529 angstroms. That is just a constant. Let's plot here the (1, 0, 0) wave function. If I went and plotted it, what I would find is simply that the wave function at r is equal to zero, here, would start out at some high finite value, and there would just be an exponential decay. Because if you look here at the functional form, what do you have? Well, you have all this stuff, but that is just a constant. And the only thing you have is an e to the minus r over a nought dependence. That is what gives you this exponential drop in the wave function. What this says is that the wave function at all values of r has a positive value. Now, what about the Psi(2, 0, 0) wave function? Let's look at that. Psi(2,0,0), or the 2s wave function as a function of r. What happens here? Well, we are plotting essentially this. All of this stuff is a constant. And we have a two minus r over a nought times an e to the minus r over 2 a nought. That is what we are really plotting here. And, if I did that, it would look something like this. We start at some large, positive value here. And you see that the wave function decreases. And it gets to a value of r where Psi is equal to zero. That is a radial node. And in the case of the 2s wave function, that radial node occurs at r equals 2 a nought. And then the wave function becomes negative, increases, and gets more and more negative, until you get to a point where it starts increasing again and then approaches zero. This part, here, of the wave function is really dictated by the exponential term, the e to the minus r over 2 a nought. This part of the wave function is dictated by this polynomial here, two minus r over ao. If you wanted to solve for that radial node, what would you do? You would take that functional form, set it equal to zero and solve for r. And so you can see that 2 minus r over a nought set equal to zero, that when r is 2 a nought, that the wave function would have a value of zero. That is how you solve for the value of r at which you have a node. Now, this is really important here. That is, at the radial node, the wave function changes sign. The amplitude of the wave function goes from positive to negative. That is important because at all nodes, for all wave functions, the wave function changes sign. And the reason the sign of the wave function is so important is in chemical bonding. But let me back up for a moment. Many of you have talked about p orbitals or have seen p orbitals before. Sometimes on a lobe of a p orbital, you put a plus sign and sometimes you put a negative sign. You have seen that, right? Okay. Well, what that is just referring to is the sign of the amplitude of the wave function. It means that in that area the amplitude is positive, and in the other area the amplitude is negative. And the reason the amplitudes are so important, or the sign of the amplitudes are so important is because in a chemical reaction, when you are bringing two atoms together and your electrons that are represented by waves are overlapping, if you are bringing in two wave functions that have the same sign, well, then you are going to have constructive interference. And you are going to have chemical bonding. If you bring in two atoms, and the wave functions are overlapping and they have opposite signs, you have destructive interference and you are not going to have any chemical bonding. That is why the sign of those wave functions is so important. So, that is Psi(2, 0, 0). What about Psi(3, 0, 0)? That is the last function, here, on the side walls. And let me just write down the radial part, 27 minus 18(r over a nought) plus 2 times (r over a nought) quantity squared times e to the minus r over 3 a nought. And now, if I plotted that function, Psi(3,0,0), 3s wave function, I would find out that r equals zero, large value of psi finite, it drops, it crosses zero, gets negative, then gets less negative, crosses zero again, and then drops off. In the case of the 3s wave function, we have two radial nodes. We have a radial node right in here, and we have a radial node right in there. And, if you want to know what those radial nodes are, you set the wave function equal to zero and solve for the values of r that make that wave function zero. And, if you do that, you would find this would come out to be, in terms of units of a nought, 1.9 a nought. And right here, it would be 7.1 a nought. The wave function, in the case of the 3s, has a positive value for r less than 1.9 a nought, has a negative value from 1.9 a nought to 7.1 a nought, and then a positive value again from 7.1 a nought to infinity. So, those are the wave functions, the functional forms, what they actually look like. Now, it is time to talk about what the wave function actually means, and how does it represent the electron. Well, this was, of course, a very puzzling question to the scientific community. As soon as S wrote down is SchrË†dinger equation, hmm, somehow these waves represent the particles, but exactly how do they represent where the particles are? And the answer to that question is essentially there is no answer to that question. Wave functions are wave functions. It is one of these concepts that you cannot draw a classical analogy to. You want to say, well, a wave function does this. But the only way you can describe it is in terms of language that is something that you experience everyday in your world, so you cannot. A wave function is a wave function. I cannot draw a correct analogy to a classical world. Really, that is the case. However, it took a very smart gentleman by the name of Max Born to look at this problem. He said, "If I take the wave function and I square it, if I interpret that as a probability density, then I can understand all the predictions made by the SchrË†dinger equation within that framework." In other words, he said, let me take Psi and l and m as a function r, theta, and phi and square it. Let me interpret that as a probability density. Probability density is not a probability. It is a density. Density is always per unit volume. Probability density is a probability per unit volume. It is a probability per unit volume. Well, if I use that interpretation, then I can understand all the predictions made by the SchrË†dinger equation. It makes sense. And, you know what, that is it. Because that interpretation does agree with our observations, it is therefore believed to be correct. But it is just an assumption. It is an interpretation. There is no derivation for it. It is just that the interpretation works. If it works, we therefore believe it to be accurate. There is no indication, there are no data that seem to contradict that interpretation, so we think it is right. That is what Max Born said. Now, Max Born was really something in terms of his scientific accomplishments. Not only did he recognize or have the insight to realize what Psi squared was, but he is also the Born of the Born-Oppenheimer Approximation that maybe some of you have heard about before. He is also the Born in the Distorted-Wave Born Approximation, which probably none of you have heard before. But, despite all of those accomplishments, psi squared interpretation, Born-Oppenheimer Approximation, Distorted-Wave Born Approximation, he is best known for being the grandfather of Olivia Newton-John. That's right, Oliver

Newton-John is a singer in Grease. Two weeks ago in the Boston Globe Parade Magazine, which I actually think is a magazine that goes throughout the country in all the Sunday newspapers, there is a long article on Olivia Newton-John and a short sentence about her grandfather, Max Born. So, that is our interpretation, thanks to Max Born. Now, how are we going to use that? Well, first of all, let's take our functional forms for Psi, here, and square it and plot those probability densities for the individual wave functions and see what we get. The way I am going to plot the probability density is by using some dots. And the density of the dots is going to reflect the probability density. The more dense the dots, the larger the probability density. If I take that functional form for the 1s wave function and square it and then plot the value of that function squared with this density dot diagram, then you can see that the dots here are most dense right at the origin, and that they exponentially decay in all directions. The probability density here for 1s wave function is greatest at the origin, r equals 0, and it decays exponentially in all directions. It is spherically symmetric. That is what you would expect because that is what the wave function looks like. You square that, you get another exponential, and it decays exponentially in all directions. That is a probability density, probability of finding the electron per unit volume at some value r, theta, and phi. And it turns out it doesn't matter what theta and phi are because this is spherically symmetric. What about the 2s wave function? Well, here is the 2s probability density. Again, you can see the probability density is a maximum at the origin, at the nucleus. That probability density decays uniformly in all directions. And it decays so much that at some point, you have no probability density. Why? Because that is the node. If you square zero, you still get zero. r equals 2 a nought. You can see that in the probability density. But then again, as you move up this way, as you increase r, the probability density increases again. Why? Remember the wave function? It has changed sign. But in this area, here, where it is negative, if I square it, well, the probability density still is going to be large. Square a negative number, you are going to have a large positive number. That is why the probability density increases right in here, and then, again, it decays towards zero. You can see the radial node not only in the wave function, but also in the probability density. Here is the probability density for the 3s wave function. Once again, probability density is a maximum at r equals 0, and it decays uniformly in all directions. It decays so much that at some value of r, right here, the probability density is zero. Why? Because the wave function is zero. You square it, and you are going to get a zero for the probability density. And then the probability density increases again. Why? Because you are getting a more and more negative value for the wave function right in this area. Square that, and it is going to increase. And then, as you continue to increase r, probability density decreases. It decreases again, so that you get a zero. You get a zero because the wave function is zero right there. This is our second radial node. But then, the probability density increases again. It increases because the wave function increases. Square that, we are going to get a high probability density, and then it tapers off. So, the important point here is the interpretation of the probability density. Probability per unit volume. The fact that the s wave functions are all spherically symmetric. They do not have an angular dependence to them. And what a radial node is. If you want to get a radial node, you take the wave function, set it equal to zero, solve for the value of r, and that gives you a zero. Now, so far, we have talked only about the probability density and this interpretation. We have not talked about any probabilities yet. And, to do so, we are going to talk about this function, here. It is called a radial probability distribution. The radial probability distribution is the probability of finding an electron in a spherical shell. That spherical shell will be some distance r away from the nucleus. That spherical shell will have a radius r and will have a thickness. And the thickness, we are going to call dr. This is not a solid sphere. This is a shell. This is a sphere, but the thickness of that sphere is very small. The thickness of it is dr. And, to try to represent that a little bit better, I show you here a picture of the probability density for the (1, 0, 0) state. This is kind of my density dot diagram. And then, this blue thing is my spherical shell. This blue thing, here, has a radius r, and this blue thing has a thickness dr. And so, I am saying that the radial probability distribution is going to be the probability of finding the electron in this spherical shell. That spherical shell is a distance r from the nucleus and has a thickness dr. Now, I want to point out that the volume of the spherical shell is just the surface area, here, 4 pi r squared, times the thickness, which is dr. Not a very thick spherical shell. The radial probability distribution is the probability of finding that electron in that spherical shell. It is like the probability of finding the electron a distance r to r plus dr from the nucleus. Why is that important? Well, because if I want to calculate a probability, what I can do then is take the probability density here, Psi squared for an s orbital, which is probability per unit volume, and I can then multiply it by that unit volume. In this case it was the 4pi r squared dr. And the result will be a probability, because I have probability density, probability per unit volume times a volume, and that is a probability. Now we are getting somewhere in terms of figuring out what the probability is of finding the electron some distance r to r plus dr from the nucleus. In the case of the s orbitals, I said that the Psi was a product of the radial part and the Y(lm) angular part. Remember that the Y(lm) for the s orbitals was always one over the square-root of one over 4pi. The Y(lm) squared is going to cancel with 4pi, and you are just going to have r squared times the radial part squared. For a 1s orbital, if you want to actually calculate the probability at some value r, you just have to take Psi squared and multiply it by 4pi r squared dr. However, in the case of all other orbitals, you cannot do that because they are not spherically symmetric. And so, for all other orbitals, you have to take the radial part and multiply it by r squared dr. I will explain that a little bit more next time. Okay. See you on Monday.